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SYMPOSIUM ON THE "ELECTRON THEORY OF SOLIDS"

EXCERPTS FROM ACTA PHYSICA SINICA

-COMMUNIST CHINA-

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SYMPOSIUM ON THE "ELECTRON THEORY OF SOLIDS" EXCERPTS FROM ACTA PHYSICA SINICA

[These excerpts include the discussions of Chinese physicists during the 11-13 January 1958 Symposium on the "Electron Theory of Solids," as reported in Wu-li Hsueh-pao (Acta Physica Sinica), Vol 14, No 3, 1958. The titles, authors, and outlines of four papers which stimulated the discussions, as well as textual matter representing the authors' own views, are given below. The original page numbers are appended at the end of each excerpt.

According to the journal, the symposium was held in Peiping by the Department of Mathematics, Physics, and Chemistry of the Academia Sinica. It was designed to impart an appreciation of important concepts which have evolved from research on the electron theory of solids conducted abroad and in China, and to stimulate the interest of Chinese theoretical physicists in this subject.

About 60 persons attended. They consisted of members of the department's committee, guests who have done or are preparing to do research on the theory of solids, and teachers. During the closing session, the group exchanged views on how to organize and develop research on the theory of solids.

Besides the four papers cited below, other papers presented at the symposium and published in this issue of the journal are as follows:

"The Present State of the Polaron Problem," by Huang K'un

"The s-d Exchange Interaction Problem in the Theory of Ferromagnetism," by Li Yin-yuan

"Recent Developments in the Theory of Spin Waves," byWu Shih-shu

"The Frohlich-Bardeen Theory of Super-Conductivity," by Ch'eng K'ai-chia.]

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HSIEH Hsi-teh

(Futan University)

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DISCUSSION

Kao Lien-p'ei* (Description of slides omitted).

Mr Hsieh spoke of the electric effect of magnetic field as one of the principal methods of measuring energy band structure. I wish to make a supplementary remark. Some interesting problems are elicited by the electric effect of a magnetic field. For instance, Justi et al. performed a seried of experiments on magnetic reluctance between 1936 and 1941.

Magnetic reluctance of single-crystal Cd[1], under the action of approximately 35 kilogausses, when the temperature is reduced from room temperature to He temperature, may increase about as high as 150,000 times (the current being nearly perpendicular to the hexagonal axis of the crystal), or may even exceed 5,000,000 times (the current being parallel to the hexagonal axis of the crystal).

Agains, in the case of magnetic reluctance of single-crystal gold[2], a very strong and symmetrical anistropic body appears when the magnetic field revolves 360 degrees around the direction of the current, which is also the direction of the cubic axis of the crystal. Though we

*Lantern slides were shown at the symposium. The remarks were made in conjunction with the explanation of the slides. The passage here was written by Mr. Kao who summarized the speech delivered at that time.

[1]Justi, E.; Kramer, J.; Schulze, R., Phys. Zs. 41(1940), 308.

[2]Justi, E., Leitfahigkeit und Leitungsmechanismus fester stoffe (Gottingen, 1948).

suggested that those problems could be decisively solved by application of the series expansion method and with the aid of a knowledge of energy band structure (a point to be treated later when the works of Lifshitz et al. are introduced), strictly speaking, however, these problems are still unsolved.

P'eng Huan-wu What do these charts signify?

Kao Lien-p'ei

As Mr. Hsieh said a moment ago, when the magnetic field is weak, energy band theory may be used to explain some phenomena of current-magnetism effect. As the magnetic field increases, the effect becomes more and more complicated. The problem of whether the effect may be explained remains unsolved. I present these charts in the hope of calling your attention to it.

Huang K'un How strong is the magnetic field here?

Is it true that the electrons may revolve many turns between collisions?

Hsieh Hsi-te

By the strong field cited a little while ago, it is basically assumed that the periodic field in which the electrons are situated is not influenced by the magnetic field. It is problematical whether it is still possible to solve Schrodinger's equation on the basis of a single electron (ignoring terms of a magnetic field) in a magnetic field as strong as 35,000 gausses.

Kao Lien-p'ei

It seems to me that a definite explanation may be given by expanding the figure [A. H. Wilson, Theory of Metals, page 318 (1953)] with the aid of Fourier's analysis into H-series. The question posed by Mr. Huang as to how many turns a free electron may revolve will probably be treated later by Mr. Chang when the works of Lifshitz et al. are introduced.

Hsieh Hsi-te Generally, ω_c is used to denote the strength of a magnetic field.

Huang K'un

Mr. Hsieh has just spoken of one type of standard. It seems to me that there is the question of two types of standards of strength: one being the comparison of the radius of orbit of motion in a magnetic field with a free path, and the other being that with the size of an atomic cell. Are they not distinct from each other in theoretical analysis?

Hsieh Hsi-te

Generally, it is more often compared with the free path. The influence of a magnetic field on the effective mass has not yet been taken into consideration at present.

Ch'eng K'ai-chia

Pekar performed some calculations on mobility of electrons in Cu_2O. One method thus employed involved computations with polarons and the other with the ordinary electrons. He affirms that the current carriers of Cu_2O are polarons. Is it not true that of the two types of cavities of germanium which you mentioned a little while ago one consists of polarons and the other is not polarized? You said that the ratio of their effective mass is 1/50. That apparently explains the above point.

Hsieh Hsi-te

It is the concentration ratio that is 1/50. The effective masses are 0.3 and 0.04 of the mass of an electron.

Ch'eng K'ai-chia

Is it not true that the electron distribution in the energy band is related to the magnetic field? For instance, Y. N. Shuvalov of Leningrad University performed electron cloud distribution on CdS with the aid of X-ray analysis and discovered that when light conducted electricity the electron cloud changed from originally strong to weak. These experiments are being continued at present, and it has been discovered that this phenomenon disapperars when

the magnetic field increases. The phenomenon is somewhat similar to the stopping of superconductance by a magnetic field in superconductivity.

Kao Lien-p'ei.

Mr. Ch'eng raised a very interesting question. What is the definition of anergy band under the action of an external field? Wannier asked this question in his work done in 1937. Recently, Slater, Luttinger, Adams et al. did some further work.

Chang Tsung-sui

Since the momentum k which comprises the vector potential is not commutative, the energy ban may possibly be meaningless (that is, the values of k_x, k_y and k_z cannot be determined at the same time).

Hsieh Hsi-te

Somebody added magnetic fiedl to the de Haas-van Alphen effect in Shrodinger's equation.

Chang Tsung-sui

How is it that the magnetic field is not altogether taken into account at the very beginning?

Huang K'un

It seems to me that this is due to a consideration of simplicity versus complexity for purposes of calculation. The periodic field is treated first, and its influence may thus simply be replaced by effective mass. However, since the kinetic energy corresponding to the de Broglie wave length involved in this method of calculation may be comparable to the distance between energy bands, then the energy bands begin to blur and the conception of an energy band becomes questionable. Perturbation correction may be applied when the difficulty is not serious.

Chang Tsung-sui

It is not a question of whether or not the energy bands blur. There are many states in an energy band, and

they are treated as continuous and denoted by k_x, k_y, and k_z. Since the magnetic field has increased in strength, momenta k's are not commutative and it is not always correct to discuss E as such and such a function of k_x, k_y and k_z, treating them as continuous. (For instance, it is not always correct to discuss the effective mass tensor through

$$\partial^2 E / \partial k_i \partial k_j .)$$

When the magnetic field is weak, this difficulty is not serious. However, as the magnetic field increases indefinitely in strength, this difficulty is bound to arise.

Huang K'un

The question is how strong should the magnetic field be.

[pages 188-189]

THEORIES ON ELECTRONIC TRANSITION IN CRYSTALS

HUANG K'un

(Department of Physics, Peking University)

I. Introduction

Photo-transition and thermo-transition

Work in earlier periods

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Configuration coordinate diagram and application of the Franck-Condon principle (Seitz-Mott theory)

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Connection of systematic theory and configuration coordinate diagram

Problems for further study

[page 191]

* * *

As to the general direction which the theory should eventually take for its further development, a clear trend has not yet emerged in contemporary scientific works. It is worthwhile to point out that there exist in contemporary theories two problems of fundamental significance which await further study.

According to Mott's theory, thermo-transition proceeds through the intersecting point of configuration curves, and the intersecting point of curves shows that in this configuration two electronic states are degenerate. The situation is similar in the theory of multiple coordinates.

The transition under high temperature takes place at least in the configuration where two electronic states are degenerate. Thus there arises a twofold question.

On the one hand, the strictly degenerate condition envisaged in theory may not generally exist in actuality. On the other hand, provided that the energy of one electronic state approaches that of another, clarification is required on the point whether the analysis on the basis of adiabatic approximation holds true.[25]

Another question concerns the transition process where electrons are captured by the impurity energy level and opposite electrons are excited from traps, which is of the highest practical significance. Calculations on this process in the past [14,25,31,32] invariably ignored the interaction of electrons in a free state with a crystal lattice.

Under general conditions, this is inconsistent with the premise of adiabatic approximation (even as an approxi-

mation of 0-degree).[15] In this sense, the current systematic theory itself is unable to take into serious consideration the situation that electronic states form a continuous spectrum.

Of course, the more clearly indicated work is to proceed further in comparing theory with experiments and to analyze the problems arising therefrom. This matter involves the analysis of effects in higher order and the study of the concrete models related to electronic states.

According to the systematic theory, for instance, if we take first approximation of the electron wave function into account, then the electric moment will include the linear term of vibrator coordinates, and the coefficient of the quadratic terms of the corresponding vibrator Hamiltonian quantity such as (4.7) will also be related to the electronic state. (That is to say, it is not solely a question of the origin of the vibrator.)

Both may cause the peak value in a spectrum to shift with temperature and may modify the shape of spectrum distribution. Moreover, the non-simple-harmonic property of crystal lattice vibration may also produce a similar result.

The solution of a number of substantial problems (such as the shape and shift, as well as the luminous efficiency, of the color center spectrum as mentioned above) is in fact reduced to the analysis of a number of such effects of higher order.

On the other hand, no matter whether it is for the purpose of performing quantitative calculations toward the solution of definite problems or to help clarify questions concerning the effects of higher order, it is always necessary to probe the problems of concrete models related to the properties of binding centers, the interaction of electrons and crystal lattices, and the definite forms of crystal lattice vibrations.

This report is based upon my general understanding of the subject. Special mention should be made that, due to haste in the preparation, it has not been possible to have some of the discussed questions and the cited data examined further and checked against original works. [page 201]

DISCUSSION

Ch'eng K'ai-chia

In a strong coupling, radiation damping plays a considerable part and should be taken into consideration; therefore, it is not possible to use $/U_{AB}/^2$ as the transition probability. Damping should be taken into account and $/U_{AB}/^2$ should be determined from the Heitler-P'eng integral equation:

$$U_{AB}=H_{AB}+\int i\pi P_e H_{AC} U_{CB} dE_C .$$

Huang K'un

Dadov did some work in which damping is taken into account. I have not made a careful study of his work and am not able to tell the definite result.

Ch'eng K'ai-chia.

The damping effect should be introduced into elements of the transition matrix. As a result of a brief consideration, we may multiply the square of the element of transition matrix by

$$\frac{(E_n-E_n')^2}{(E_n-E_n')^2+\Gamma^2}$$

It is directly proportional to a factor

$$e^{-\frac{(E_n-E_n')^2}{\sigma}}$$

Thus, the maximum value of transition probability is not at $E_n-E_n'=0$. This may explain the shift with temperature of the peak value of the color center. According to my calculation, the shift $\propto T^{\frac{1}{2}}$.

Huang K'un

As the actual result, it is basically directly proportional to T.

Ch'eng K'ai-chia

Your original method can be used only for long waves. The change in w concerns short waves. The method is not applicable here, because the recoil between phonons has not been considered.

P'eng Huan-wu

Does the method in question mean the adiabatic approximation?

Ch'eng K'ai-chia

The one used is a contact transformation similar to that of Bloch-Nordsieck. It is tantamount to neglecting the action between phonons.

P'eng Huan-wu

It is a question of the origin moving.

Huang K'un

I still do not understand how there is a question of recoil here.

Ch'eng K'ai-chia

The situation is tantamount to combining the term of interaction $qk'e^{ik.x}$ of square matching. A is related to x. This method is the Bloch-Nordsieck method with the recoil omitted. It is due to this fact that the L. L. P. polaron has been criticized for providing no consideration for recoil afterwards. It is considered in an approximate member.

Huang K'un

It seems that this problem will not arise if adiabatic approximation may be used.

Ch'eng K'ai-chia

That is the point, but adiabatic approximation cannot be used.

Huang K'un

Generally speaking, recoil presents no difficulty in the problems of bound electrons, because the localized wave function comprises all the momentum states and may absorb random recoils. Secondly, in this connection, it is not a question of emission of phonons by electrons, but of the change of the elastic equilibrium point so that there is a release of elastic energy appearing in the form of phonons and so that the total momentum of the released phonons is 0. [pages 202-203]

THE THEORY OF COLLECTIVE VIBRATION OF ELECTRONS

Ch'eng K'ai-chia
(Nanking University)

I. Introduction

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2. Electron gas density

3. Two types of fluctuations: thermal motion and collective vibration

4. Interaction of high-speed electrons and collective vibrations

III. Quantum theory

5. Demarcation between collective vibration and individual motion of electrons

6. Representation with interaction between plasma vibration and electron eliminated

7. Determination of K_D, correlation energy

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8. Wolff-Adams theory

9. Theories of Frohlich, Hubbard, Mott, et al.

10. Interaction of ionic vibration and electronic collective vibration and its Hamiltonian

11. Hamiltonian of electronic and ionic vibrations after the elimination of interaction

12. Problem of interaction of a particular electron and ionic vibration.

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* * *

VI. SOME CONCLUDING REMARKS

The study of the question of multiple electrons in metals with the aid of the concept of collective motion of electrons is indeed a great leap forward in theory. Basically, it solves the problem of potential energy of interaction between electrons in metals, elicits the existence of collective macroscopic motions of electrons, and shows the demarcation between microscopic and macroscopic motion.

This theory is substantiated by both the theoretical and experimental points of view. Moreover, there has been progress in mathematical technique in the theory itself, and it is possible to consider concrete problems and to compare experimental data. It is also possible to predict the existence of discontinuous energy levels of collective vibrations. Therefore, it is possible to ascertain that this effect does exist.

However, there are a few questions in the theory itself which deserve more thorough investigation.

1. The question of collective motion in a full band or a nearly full band should studied more thoroughly. It is necessary to study how the influence of the energy band on collective vibration manifests itself in this key question,

and to study whether there is shielding action in a full band and how the shielding action of different energy bands takes place.

Particularly, it is necessary to study how the distribution of electrons between various energy bands is related to the frequency of vibrations.

2. Is there any more appropriate rule for the choice of K_D? The rule for solving for K_D by minimizing ξ" relying on the variational theory, cannot be accepted as the rule for determining the physical K_D, but is only a rule of convenience, and thus the physical significance of Debye's wave length for K_D is not sufficiently clear. Moreover, K_D^{-1} in metals is far smaller than the distance between atoms and its influence on atoms must be given careful consideration. In fact, this is the influence of an energy band and a deeper understanding of it is necessary.

3. Study should be made of the region where $\omega_0^2 < \Omega_0^2$ because the condition $\omega_0^2 < \Omega_0^2$ is similar to the basis on which Wentzel objected to the Frohlich-Bardeen theory in superconductivity.

4. As to the accuracy of the calculation of binding energy, application of the Bohm-Pines theory is not appreciably more successful than that of the Wigner-Seitz method. Therefore it is necessary to study the methods in order to achieve accuracy.

In addition to the above, in connection with the course which the development of the theory of collective vibration may take, there are several problems that may be investigated. For instance:

1. We study the canonical transformation

$$U = e^{\frac{i}{\hbar}\int \xi_{\text{inter}}\, dt}$$

This is opposite to the interaction representation of Tomonaga Shinchiro and may be termed the "Actionless Representation." What are the characteristics of this transformation? Is there any general theory to be introduced?

2. In electrodynamics collective vibrations may also occur in electrons of negative energy levels. It is true that their frequency apporaches infinity, as

$$\omega^2 = \frac{4\pi e^2 n}{m}, \quad n \to \infty$$

However, study may be made with the aid of the technique of positive reduction. The question is: What do those vibrations manifest in the field theory? Is there any new subject matter?

3. What is the interrelation between ionic vibrations and electronic vibrations? Since there are polarons in ionic vibrations and also in electronic vibrations, in what transitional form does the fluctuation of those two types of polarons cross over from one type to the other? Is there a transitional parameter? Where is the transitional point? Has it anything to do with superconductivity?

The above are some of the problems I suggested. The solution of those problems will be helpful toward an explanation of many phenomena in metal-semiconductors and ionic crystals, may also reveal the characteristics in new crystals, and may perhaps solve the problem of superconductivity.

[pages 259-260]

* * *

DISCUSSION

P'eng Huan-wu

I do not sufficiently understand the area which λ_D may define. The area which may be defined by ρ will be larger than that by λ_D. Is λ_D related to the mean distance between background positive charges? Is λ_D larger or smaller than it?

Ch'eng K'ai-chia

From the point of view of the theory itself, they should be related. If λ_D is smaller than the distance between atoms, then the average positive charge distribution will be meaningless. In principle, λ_D should be larger than the distance r_s between atoms. However, as a matter of fact, $\lambda_D \sim 0.6$ Å and $r_s \sim 3$ Å for metals. Indeed, the question of an energy band is involved here, for $k\omega$ is very large and energy band structure will definitely be involved.

Chang Ch'eng-hsiu

Recently a paper by Ichikawa on electronic collective motions is solids was published (Ichikawa, Y. H., Prog. Theoret. Phys. 18 (1957), 247). He did not employ the method of canonical transformation used by Bohm and Pines, but defined the coordinates of electronic collective motions by the fluctuations of electron density. His method has the following merits: (1) It may avoid the difficulty caused by the introduction of auxiliary conditions; (2) it may be applied to other forms of potential energy than the Coulombian potential; (3) it takes into consideration the periodic field in solids; (4) it treats the kernel electrons of ions and valence electrons similarly, and therefore the polarization effect of an ionic kernel may be discussed. (5) Owing to the use of second quantization, the property of Fermi statistics of electrons has been taken into consideration.

Ch'eng K'ai-chia

Bohm and Pines also worked with second quantization and then Heisenberg representation. Usually we hope to make use of the Hamiltonian.

Yang Li-ming

It makes no difference in the application of canonical transformation whether the second quantization is used. The Japanese have a set of methods of their own in introducing collective motion.

The collective motion in an atomic nucleus is an another form. It seems to me, therefore, that the statment in the

report that the theory may offer the possibility of solving the problems in this respect might not have any foundation.

Chang Ch'eng-hsiu

In some nuclear excited states corresponding to volume vibrations, it is possible to apply such a description of collective motion to the nucleon in the nucleus (Ferentz, M.; Gell-Mann, M.; and Pines, D., Phys. Rev. 92 (1953), 836). However, it is surface vibration in the case of a low-energy nuclear state that is more easily excited. The description given above of collective motion may not be applied to nucleons under that condition (Pines, D., Solid State Physics, Vol 1, 1955, page 449).

Chang Tsung-sui

If the Hamiltonian with the form of E^2 in electrodynamics is not satisfactory, we may consider directly the interaction between electrons and ions, using second quantization. Auxiliary conditions may be avoided in this way. In quantum theory, the division of H into

$$\lambda > \lambda_0 \quad \text{and} \quad \lambda < \lambda_0,$$

and thus into collective and individual motions, appears to be the play of trial-and-error in order to get the answer because the original Hamiltonian and the auxiliary conditions are both independent of λ_0.

It seems to me that the most essential factor hinges on the criterion of the division of those two types of motions--collective and individual. In this respect I do not agree completely with the classical part. The criterion for distinguishing the collective and individual motions ρ and η is not whether η and ρ may satisfy a single equation. The difference between the individual part ρ_1 of ρ and the original ρ in theory consists only in that a similar shielding is added to each electron. Therefore, η should be able to be divided into two parts--the collective and the individual; thus there is also a collective component in η.

The theory of division into two types of motions does not only originate from Newton's formula, but should also concern the correlation between two electronic motions, which is to be used as such a criterion.

Huang K'un

I wonder if the justification of λ_D consists in that it is actually possible to make the term of individual motion in the part of collective motion, as well as the term of collective motion in the part of individual motion, very small. It seems that the purpose of the variational method is to make setting those terms at minimum the most appropriate method of choosing the demarcation point λ_D. Of course, the demarcation between those two cannot possibly be absolutely rigid.

In connection with the interpretation of the Bohm-Pines theory, I wish to add an idea of my own. The interaction between electrons had in the past been represented by an average field. Apparently, an average field had not solved the problem of interaction, because, as a result of taking the solution in an average field as an approximation of 0-order and then taking interaction as perturbation, the difficulty of divergence arises. Bohm and Pines solved that problem from an entirely different angle, because the collective vibrations with very high frequency under general conditions do not excite electrons which are acted upon by the remaining so-called individual motions as if there are Coulombian forces.

Therefore, a solution has been found for the assumption made in the past that electrons are basically treated as free electrons. Free electrons, though not entirely unshielded exhibit only shielding Coulombian forces among themselves (thus greatly reducing the short-distance action). Vonsovsky pointed out that one of the purposes of the study of the theory of multiple electrons is to show how the single electron theory succeeds so triumphantly. I feel that the Bohm-Pines theory has basically achieved that.

Ch'eng K'ai-chia

λ_D may be treated as a variable parameter in the ordinary variational method. Variation makes the first approximation a minimum.

Li Ying-yuen

No mention has been made in experiment or in the theory as to whether it is possible to excite plasma vibration with electromagnetic waves. I wonder if Mr. Ch'eng has examined this problem.

Ch'eng K'ai-chia

I have not. Pines did reveal that an electromagnetic wave could not excite vibrations when passing a metal plate which was too thin.

Huang K'un

In connection with an electromagnetic wave, is it not necessary to consider the transverse wave? The frequency of transverse waves is lower. I wonder how low it is.

Ch'eng K'ai-chia

It is of the same order of magnitude.

Chang Ch'eng-hsiu

On the blackboard Mr. Ch'eng wrote q as the vanishing operator of the longitudinal wave photon in the longitudinal wave expansion of A, and later on q appeared again in H as the collective vibration coordinate.

Ch'eng K'ai-chia

Both a^- and a^+ are included in q.

Chang Ch'eng-hsiu

My question is whether or not the plasmon may be treated as a longitudinal wave photon.

Ch'eng K'ai-chia

Yes, it may.

P'eng Huan-wu

But connections may be made between this longitudinal wave photon and the auxiliary conditions, while a large portion of the problem cannot be seen if it is placed under the auxiliary conditions.

Chang Tsung-sui

This is one of the unique specifications of the electromagnetic field: $\phi = 0$ and $A \neq 0$, which is just opposite to that in the method used in ordinary quantum electrodynamics.

[pages 260-261]

A BRIEF ACCOUNT OF THE RESEARCH WORK OF N. N. BOGOLIUBOX AND OF N. M. LIFSHITZ

Chang Tsung-sui
(Institute of Mathematics,
Chinese Academy of Sciences)

The report is divided into three parts. One part concerns the approximate theory of second quantization of Bogoliubov (with an additional description of the method he used in treating the perturbation theory of the degenerate system). Another part relates the main points of his paper on the superconductivity theory. The third part gives an account of Lifshitz's work in the study of the properties of metals under a magnetic field. The last part is to be supplemented by Comrade Kao Lien-p'ei.

[page 274]

DISCUSSION

Hsieh Hsi-te

The Lifshitz theory described by Mr. Chang has much to contribute to the study of the de Haas-van Alphen effect in metals. The resulting quantization condition

$\oint P_y \, dp_x = (n + r)k\frac{2\pi eH}{c}$ is the same as that obtained by Onsager[1]. By measuring the period of the oscillation of magnetization, $\oint P_y \, dp_x$ may be solved.

[1] Onsager, L., Phil. Mag. 34 (1952), 1006.

The effective mass of the closed surface of equal energy mentioned by Mr. Kao may be expressed as

$$m^* = \frac{\hbar^2 \partial S}{2\pi \partial E} .$$

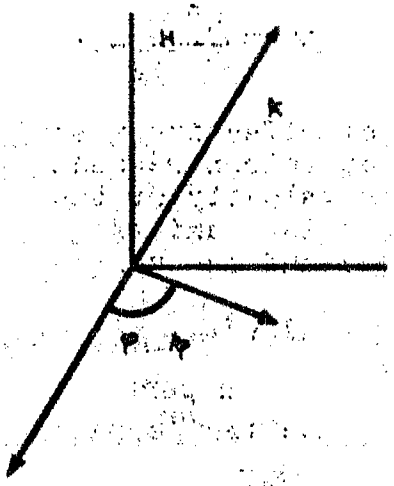
In fact, this form of effective mass has been adopted in the experiments on cyclotron resonance of p-type germanium and silicon. If the velocity of the cavity perpendicular to the magnetic field is v and the momentum perpendicular to the magnetic field and the velocity is p, then $dp = \frac{e}{c} vH\, dt$.

$\frac{2\pi}{w} = \oint \frac{c\, dp}{eHv}$ and $v = \hbar \frac{\partial E}{\partial K_\rho}$, where k_ρ is the component of vector k in the direction perpendicular to H. From

$$w = \frac{eH}{m^* c}$$

and $dp = k_\rho\, d\varphi$, we obtain $m^* = \frac{\hbar^2}{2} \oint \frac{k_\rho\, d\varphi}{\frac{\partial E}{\partial K_\rho}}$. If $\frac{\partial E}{\partial K_\rho}$ is independent of φ, then the above equation becomes the same as

$m^* = \frac{\hbar^2 \partial S}{2\pi \partial E}$. From the study of the change with temperature in the oscillating amplitude of magnetization in the de Haas van Alphen effect, m* may be determined.



Moh Tang

Having heard Mr. Chang Tsung-sui's and Mr. Kao Lien-p'ei's accounts of the theory on galvanic phenomena of a magnetic field in metals advanced by I. M. Lifshitz et al., I wonder if it is possible to give a more configurationized interpretation to the theory in a rudimentary way.

Lifshitz et al. clearly and definitely pointed out that two types of energy-quasimomentum (E-p) relations of electronic states in metals should be distinguished, that is to say, the two types of surfaces of equal energy in quasi-momentum space should be distinguished. Figure 1 is a two-dimensional diagram indicating the two conditions

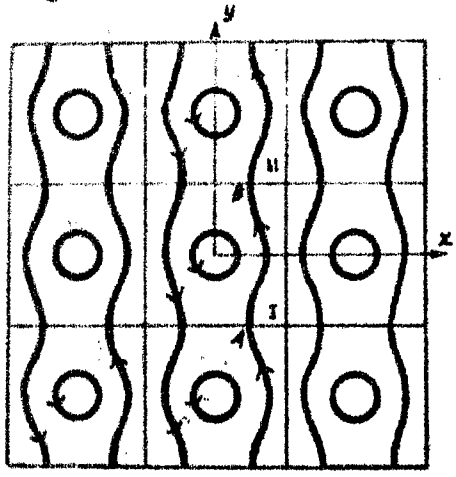


Figure 1

distinguished by Lifshitz et al. In the figure, A represents a non-closed surface of equal energy. What is the fundamental difference between those two cases?

According to the accounts given by Mr. Chang Tsung-sui and Mr. Kao Lien-p'ei, in the case of a closed surface of equal energy, when there is the action of an external magnetic field, the quasimomentum p of electrons moves along a closed curve (the curve of intersection of the plane perpendicular to the external magnetic field with the surface of equal energy), returning to its original position in a definite period without cessation; therefore the effective mass m* may be positively defined by the period T.

In a non-closed surface of equal energy, however, p may extend toward infinity along the non-closed curve, without returning, and therefore m* cannot be defined in the same way. The two forms of motions of p are indicated by the arrows in Figure 1.

It seems to me, however, that $\mathcal{E} = \mathcal{E}(p)$ must also be periodic, considering the periodicity of a crystal lattice. Therefore area I is physically the same as area II, and point A is physically the same as point B. When p goes from point A to point B, it is tantamount to its returning to point A and repeating hereafter the motion along line AB without cessation. Thus, in the case of a non-closed surface of equal energy, the motion of electrons in p space is still periodic as in the case in a closed surface of equal energy. It is not necessary to envisage it as extending to infinity.

In line with the idea that occurred to me just a little while ago, I wonder if it is possible to view the intrinsic difference between the two situations from the standpoint of symmetry. Since the periodicity of $\mathcal{E} = \mathcal{E}(p)$ has already been mentioned above, it is only necessary to examine the surfaces of equal energy below (Figure 2 and Figure 3). The shaded areas represent the electrons in the vicinities of Fermi surfaces. The energy levels within the Fermi surfaces are almost all occupied by electrons. It may be seen from Figures 2 and 3 that the distribution of electrons is symmetrical, both with respect to a horizontal axis and to a vertical axis.

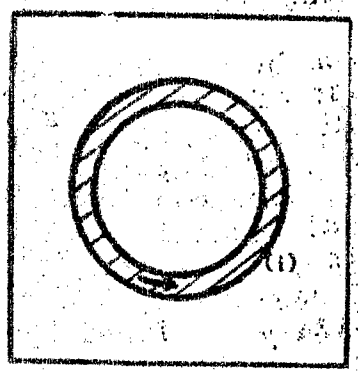


Figure 2.

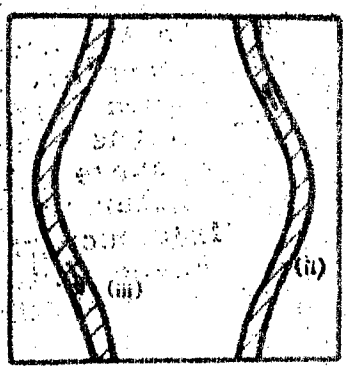


Figure 3.

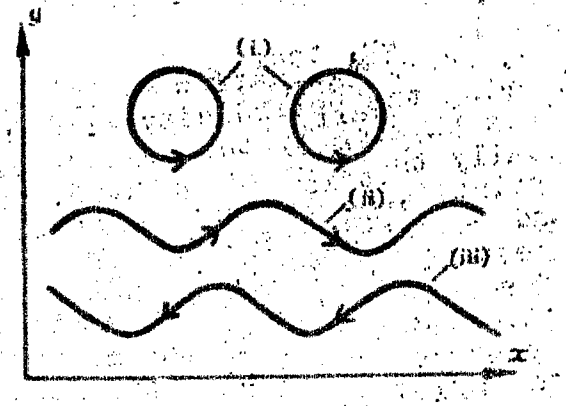


Figure 4.

Under the action of the magnetic field H_z in a direction perpendicular to, and away from, the plane of the figure, the electrons move in the p space only along the surfaces of equal energy (represented by the curves in the figures). The senses of direction of the motions are indicated by arrows. As to the motions in ordinary space of the corresponding electrons under those two different conditions, indication is made diagrammatically in Figure 4.

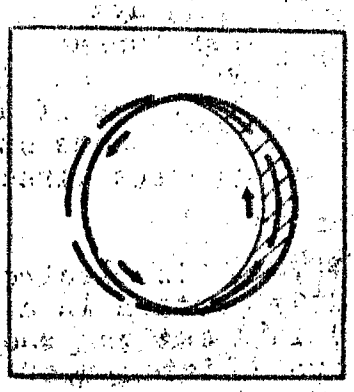


Figure 5.

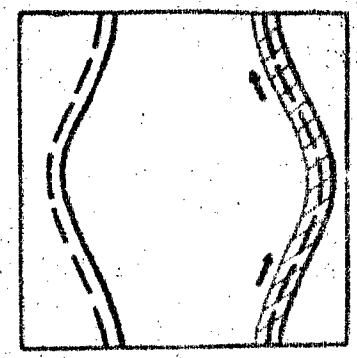


Figure 6.

Then the influence of the strong magnetic field on the electronic directional motion produced by the action of an electric field is the same as that caused by revolving the shaded area in Figure 5 around the origin in circles. Thus the electronic directional motion no longer maintains a definite direction, but takes all directions, and if viewed in the entirety it is completely cancelled.

Very clearly, the electrons in a closed surface of equal energy, such as (i) are always travelling in circles. Some electrons on a non-closed surface of equal energy, such as (ii), however, have moved in the direction of x for a length of path after the lapse of an interval of time. At the same time there must be some other electrons such as (iii), moving in the opposite direction (the direction of -x).

Therefore, as far as all electrons in the entirety is concerned, there is no motion in a fixed direction. Here, if the magnetic field is strong enough, then, in the time interval between two collisions of electrons, the number of turns an electron in Figure 2 revolves will be the same as the number of times an electron in Figure 3 repeats its motion.

If the action of an electric field is introduced in addition to that of the magnetic field, the situation will be different. We may view it in the following way. Figure 5 and Figure 6 represent the situations where only electric field is applied. Under the action of the electric field, the entire electron distribution moves along the direction of the electric field in the p space. At the same time, due to occurrence of collisions which cause them to return to their original distribution, stable distributions such as shown in Figures 5 and 6 are thus reached. These distributions are not symmetrical.

The parts remaining after the symmetrical components have been taken away are represented by the shaded areas in the figures. This corresponds to the fact that the motion of some electrons in ordinary space cannot be offset by the motion of other electrons in the opposite direction. Hence, in both cases of the two types of surfaces of equal energy, there are directional motions of electrons. In other words, electric current is produced.

When a magnetic field also exists at the same time, the action of the magnetic field will cause the electrons to move along the surface of equal energy in the way described above. In the case of a closed surface of equal energy, we envisage a spherical surface of equal energy, that is, the area occupied by an electron revolving on the xy plane with the origin as the center.

It is the same as revolving fan blades and appears to be a circular disc. As far as the motion of electrons in actual space is concerned, the individual electrons situated in the shaded area in Figure 5 at that time, acting as (i) in Figure 4, are not proceeding uniformly in a certain direction. A conclusion[1] may thus be reached that in the metals whose Fermi surfaces are closed surfaces of equal energy, as the magnetic field H_z increases to a considerable magnitude, the current (that is, the conductance) perpendicular to the direction of the magnetic field approaches zero.

In the case of a non-closed surface of equal energy, the influence of the magnetic field on conductance is entirely different. The action of the magnetic field causes the electrons to travel along the surface of equal energy in the p space. As may be seen from Figure 6, although the electrons in the shaded area may travel back and forth, they will remain in the vicinity of the shaded area (moving in the direction as indicated by the arrows in the figure).

Therefore, the directional motion of the electrons produced under the action of the electric field, as represented by the shaded area, still exists. Therefore, the electric current does not disappear and the situation is generally similar to that without the magnetic field.

With more specific reference to the situation in the actual space, the electrons moving as (ii) in Figure 4 will exceed those moving as (iii), with the result that directional motion cannot be cancelled completely. It may thus be seen[2] that in the metals whose Fermi surface is a non-closed surface of equal energy, as the magnetic field H_z increases to a considerable magnitude, the conductance in the direction of x will not approach zero but will actually approach a stable value.

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[1] Note after the Conference: This point was not expressly brought out when the speech was delivered. Later on, Mr. Huang K'un supplemented my idea.

[2] Same as 1.

In short, to summarize the above analysis, the difference of the two types of surfaces of equal energy lies in the difference in symmetry. In a plane perpendicular to the external magnetic field, the electrons on the closed surface of equal energy can travel continuously along the surface of equal energy to a position symmetrical with respect to the origin of the p space, while the electrons on the non-closed surface cannot.

Though the two points symmetrical with respect to the origin of the p space possess the same energy, however, they are on different branches of the intersecting curve of the surface of equal energy and the plane perpendicular to the external magnetic field; therefore, they cannot cross over continuously along the interesecting curve.

It may be seen from the results that the mean velocities under the action of an electric field and a strong magnetic field are different for electrons with different types of surfaces of equal energy as their Fermi surfaces. If the surface is closed, the velocity is almost equal to zero. If the surface is non-closed, it is not so in certain directions.

The above is an attempt to explain the physical aspects of the theory of Lifshitz et al. in a more intuitive and simplified manner. Of course, the rigorous theory which describes the actual situations is far more complicated and involves many more problems.

In addition to the introduction, with much emphasis, of the most significant concept of the necessity of distinguishing the two types of surfaces of equal energy, Lifshitz et al. also threw further light on the Boltzmann equation and performed calculations on conductivity, without any assumption of the concrete form of the surface of equal energy and of the collision mechanism.

Their findings, if compared with the experimental results, should furnish information on electron energy band structure. However, there has not yet been any definite work along this line. There has been considerable progress on formulating a phenomenalogical theory on different phenomena of transition of electrons under the action of an electromagnetic field. At the same time, some of the new advances in experimental technique are eliciting increasingly more useful data.

It is of great importance to coordinate those two phases of work, in order to study the concrete states of electrons in metals. I understand that the work of Lifshitz et al. is precisely of this nature. I have not read the full texts of the papers by Lifshitz et al., but only the abstracts of some of their work.

I know that, in addition to the theories cited at this conference, they also did much work on theories of solids and metals, for example, in the field of galvanomagnetic phenomena in metals, the influence of the quantum effect and of the Fermi energy level change etc., as well as cyclotron resonance in metals, some magnetic resonance phenomena, the skin effect, and other macroscopic theories and crystall lattice theories related to the electromagnetic field in metals.

Ch'eng K'ai-chia

I wish to submit a supplementary account to Bogoliuboy's theory on superconductivity, Bogoliubov made a contact transformation of the generating and vanishing operators

a_k^+, 1/2 and $a_{k'}$,-1/2 of the electrons:

$$a_{k_0} = u_k a_{k,1/2} - v_k a^{+}_{k,-1/2},$$

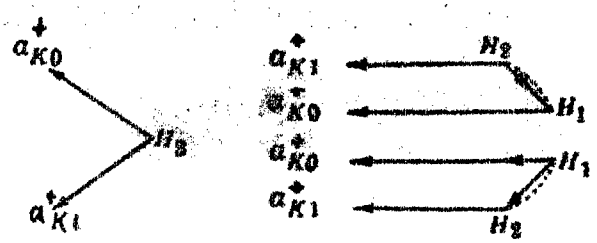
$$a_{k_1} = u_k a_{-k,-1/2} + v_k a^{+}_{k,1/2},$$

$$u_k^2 + v_k^2 = 1.$$

This transformation is tantamount to making a linear combination of the wave function of the electrons, so that the energy level may be adjusted. However, such a transformation will cause the new Hamiltonian to contain terms with

$a_{K0}\, a_{K1}$ or $a^{+}_{K1}\, a^{+}_{K0}$.

Those terms will cause divergence at the first perturbation. Bogoliubov applied one condition to determine u_k, v_k, so that the sum of the elements of the transition matrix in the following form may equal zero:



There may be two different sets of (u_k, v_k), one set being the old Fermi distribution $(u_k, v_k) = (1,0)$, and the other being the new distribution:

$$u_k^2 = \frac{1}{2}\{1 + F(k)\}, \quad v_k^2 = \frac{1}{2}\{1 - F(k)\},$$

where F(k) is a function of k, and when $k - k_0$ (the value of k on the Fermi spherical surface),

The total energy of the new distribution (in unit volume) is lower than that of the old Fermi distribution,

$$|F(K)| \rightarrow 1$$

where g is the coupling constant, $N(\mathcal{E})$ is the energy level density on the Fermi surface and ω is the frequency of ionic vibration. This distribution is known as the basic state, which describes the state of superconductivity.

Bogoliubov also showed that the energy required to excite one electron out of the basic state is at least

$$\Delta\mathcal{E} = \hbar\omega e^{-1/P}$$

Energy between the excited state and the basic state is not continuous. That is precisely the condition that superconductivity may produce permanent current.

Huang K'un

Yesterday I exchanged some ideas with Comrade P'eng Huan-wu on the subject matter of the Conference. We have some views in common. I wish to take this opportunity to express some of my feelings on the content of our talk.

A special feature of the reports to the Conference is that more emphasis is placed on some topics where theoretical work is concentrated. Therefore it is necessary for us to take notice of the fact that the theory of solids is not included in its entirety.

At the same time, there are two aspects which should be stressed. In the first place, the problems being worked on today in different countries are not necessarily those requiring most attention. If we have not yet obtained a firm understanding of some comparatively older fields, it is imperative for us to do so with urgency and dispatch, according to the needs of our own program. On the other hand, one of the most essential tasks in expanding theoretical work in this field is to coordinate it with experimental work and to meet the needs of further development.

It seems to me that the above two aspects concerning the fulfillment of our actual objective must be given special consideration when we evaluate the significance of the various problems reported here.

Hsieh Hsi-te

I wish to give a short account of some work on the bound state of electrons in solids studied with the aid of spin resonance absorption, mainly in connection with an F center. An F center is produced by the presence of negative ionic vacancy in halides of alkaline metals. It is tantamount to a center of positive electricity and may bind the electrons moving in its vicinity. The following results have been obtained in the study of the electron spin resonance absorption of an F center:

1. Shift of factor g. The energy level of a free particle whose spin is S will split into (2S + 1) levels in a magnetic field. The distance between levels is $g\mu_B H$, where g is the well-known factor g. If a high-frequency magnetic field with a vertical frequency ω is applied in addition to the static magnetic field, and if the frequency satisfies the following condition:

$$\hbar\omega = g\mu_B H \quad (1)$$

(where μ_B stands for Bohr magneton), then the particle may absorb energy from the high-frequency field and produce a transition between levels. Thus g may be determined from a measurement of high-frequency power absorption. As there is only one electron bound in the vicinity of the negative ionic vacancy and it is moving, the spin is 1/2 and g should be 2.0023.

However, it is found from the study of F center spin resonance absorption in KCl that $g = 1.995 \pm 0.001$. Then $\Delta g = -0.007$, and this is known as the shift of factor g. It is generally believed that the shift may possibly be due to the coupling of the spin with the orbit, and therefore it may be deduced that the wave function of an F center certainly contains the component of $l \neq 0$. To interpret the shift of factor g, the following assumptions have been made concerning the wave function of an F center:

(1) In addition to the potential field of the negative ionic vacancy, which acts as a positive electricity center, there is also the influence of the potential field

of the six surrounding K^+ ions. Therefore, the potential field is not in spherical symmetry and the basic state does not necessarily consist only of the function of $\ell = 0$. If the potential field is in cubic symmetry, the basic state may contain components both of $\ell = 0$ and of $\ell = 4$. Calculations show that it is necessary to assume the component of $\ell = 4$ at a considerable magnitude, in order to give Δg a satisfactory interpretation.[1]

(ii) Another approach is to express the wave function as the linear combination of the wave functions of the six alkaline metal atoms with K^+ ions as the centers. Due to polarization resulting from the existence of the negative ionic vacancy, the wave function of the basic state contains components s and p. Assuming that the component of function p is comparable to that of function s, then Δg obtained from experimentation may be interpreted.

2. Width of the line of spin resonance absorption. The experiment with KCl shows that the width of absorption line is $\Delta H = 56$ oersteds and the form is that of a Gaussian curve. If the width of the line is thought to be caused by the spin-spin interaction between the F center electrons, then for crystals with an F center concentration of $10^{18}/cm^3$, the width of the line can only be $\Delta H \sim 10^{-2}$ oersteds and the form of the line will be similar to that of the Lorentz absorpiton curve. This serves to explain that it is impossible to interpret the width of the line of F center spin resonance absorption with the aid of the spin interaction between the electrons. It is now believed[1] that it is caused by the superposition of the superfine interactions of nuclear magnetic moments of electrons and the six K^+ ions.

If the F center electron is envisaged to move in the vicinity of K^+ for a considerable interval of time, the magnetic moment of the nucleus of K is $I = 3/2$, possibly in four positions. Considering that there are six K^+ ions, we see the possibility of $4^6 = 4096$ forms for the position of nuclear magnetic moment. The distribution of these

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[1] Kohn, A. H.; Kittel, C., Phys. Rev. 89 (1953), 315.

[1] Kip, A. F.; Kittel, C.; Levy, R. A.; Partis, A. M., Phys. Rev. 91 (1953), 1066.

positions is in Gaussian form, and therefore the absorption curve is also in Gaussian form. The energy of superfine interaction may be expressed in the following way:

$$H = \sum_i a_i \mathbf{S} \cdot \mathbf{I}_i \qquad (2)$$

$$a_1 = -\frac{16}{3} \frac{\pi \mu_B \mu_n}{I} |\psi_i| \qquad (3)$$

where μ_n stands for magneton of potassium nucleus and ψ stands for the value of electron wave function at the atomic nucleus of K^+ ions. Hence it may be seen that the pattern (ii) described above in connection with wave function is more appropriate, if viewed from the angle of interpreting the width of the spin resonance absorption line.

In natural KCl, there are 93.08% of K^{39} and 6.91% of K^{41}, and $\mu_{41}/\mu_{39} = 0.55$.

Therefore, the width of the spin resonance absorption line should be smaller for $K^{41}Cl$--being $\Delta H \sim 31$ oersteds as obtained from theoretical calculation--although it is obtained experimentally that $\Delta H \sim 36 \pm 2$ oersteds for $K^{41}Cl$.

In order to interpret this result, it is assumed that the electrons not only move in the vicinity of K^+, but also may move in the vicinity of the neighboring Cl^- and may produce a superfine interaction with the Cl^- nuclear magnetic moment. The above experimental result may serve to explain that the electrons of the F centers are not localized in the vicinity of negative ionic vacancies, but enjoy greater freedom of motion.

It may be seen from the above that the experiments on electron spin resonance absorption are helpful to an understanding of wave function of an F center. Moreover, from the study on the electron spin resonance absorption in n-type silicon[2], the energy level splitting due to the superfine interaction of nuclear magnet moments between electrons and donor impurities has also been obtained. The

[2]Luttinger, J. M.; Kohn, W., Physi Rev. 97 (1957), 883.

value of the electron wave function at the position of the atomic nucleus of donor impurity may be obtained from a study of the distance between absorption spectrum lines.

Chang Ch'eng-hsiu

Is it not possible that the magnetic moment interaction of the electron with the neighboring Cl^-, as mentioned by Mr. Hsieh, is the interaction with the adjacent quadrupole moment?

Hsieh Hsi-te

The question of the action with quadrupole moment has not beeen considered.

Kao Lien-p'ei

What problems have been solved by Bogoliubov's theory? For instance, some problems are mentioned by Feynman in the recent issue of the Modern Physics Review (April 1957): specific heats of superconductors; the fact that superconductors are not simple elements, but mostly the elements in the middle rows of the periodic table; the relation between superconducting alloys and their constitutents, since some alloys are superconductors although none of the constituent elements of such alloys are superconductors; the relation between superconductivity and crystal structure, as some elements may become superconducting in certain structures but may not become superconducting in other structures; etc. Are those questions considered in Bogoliubov's theory?

Ch'eng K'ai-chia

Bogoliubov's conclusion is that all conductors may show superconductivity, irrespective of their structures.

Kao Lien-p'ei

According to his theory, which is more fundamental? Total diamagnetism of permanent current?

Ch'eng K'ai-chia

Yes, permanent current. I wish to raise a question in connection with magnetic resonance. Is it possible to solve for $|\varphi|^2$ with the nuclear magnetic moment resonance?

Hsieh Hsi-te

φ is studied with the aid of interaction between electrons and nuclear magnetic moments.

Kou Ch'ing-ch'uen

I agree to the views expressed by Mr. Huang K'un a little while ago. A comprehensive study should be made of the theory of solids. Different methods must be used for different kinds [of solids]. The electron theory has been stressed in this symposium, but this does not mean that the electron theory is of exclusive importance. Our program should not be confined to this field in its further expansion.

The methods of study of solid theory in the past generally were of two extremes. One was to emphasize electrons and to overlook atoms; the other was to concentrate on atoms and to ignore electrons. We may as well try to explore the possibility of establishing an over-all method which emphasizes both the electrons and the atoms.

It seems to me that we should devote attention to the introduction and extension of the use of methods of quantum chemistry in studying solids. The study of solids by means of methods which rely on atomic structure, molecular structure, and chemical bonds may unite the problem of atoms and molecules with theories on solids. Some researchers have some work in this field, for instance, L. Pauling, who advanced the theory of metal bonds. However, his theory is still in the qualitative stage. We should examine whether this theory may be explored and developed further. Moreover, the work of P. Lowdin is also noteworthy.

Li Ying-yuen

Basically, I share the view that it is necessary to take into consideration research based on using the atom as the unit, as brought out by Mr. Kou Ch'ing-ch'uen.

To cite an example, the problem of the ferroelectric property of the $BaTiO_3$-type is not easy to approach by starting directly from the electron theory.

Besides the treatment in thermodynamics, which is very successful, there are some rudimentary theories which consider the question with the aid of chemical bonds. Another example is the case of the case of the antiferromagnet and ferromagnet. If studied exclusively from the point of view of superexchange action, then certain phenomena, such as the change in symmetry of crystal structures, will be very hard to explain.

The theories of solids may be classified into three types: (1) the theory based on electrons, (2) the theory based on atoms, and (3) the theory based on a plastic (continuous) medium. The subject discussed in this conference is the part with the most abundant and the most systematic materials, but it is not complete as such.

Ch'eng K'ai-chia

I share Mr. Huang K'un's view that we should not concentrate solely on the field theory. It should be taken as only one of the methods. Theories on impurity, holes and displacement in the study of solids are mainly concerned with industrial application. Primary emphasis should be given to research work on atomic impurity, holes,and displacement. We should not exert too much effort to work in the field of electron theory of solids. It is wrong to work in this field exclusively.

Huang K'un

I understand that the Department [the Department of Mathematics, Physics and Chemistry, a branch of Chinese Academia Sinica] hopes to be able to hold small symposia like this one on a more permanent basis hereafter, mainly for the purpose of improving our understanding of some specialized field. In order to be more thorough, the scope of the subject of each symposium should not be too broad. The subject of this symposium is not the theory of solids, but the electron theory of solids.

[Pages 283-288]

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